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HIGH SPEED NUMERICAL INTEGRATION OF FERMI DIRAC INTEGRALS

by

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HIGH SPEED NUMERICAL INTEGRATION OF FERMI DIRAC INTEGRALS

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ABSTRACT

In this thesis we present an algorithm for the precise determination of Fermi-Dirac (FD) integral functions, $f_\tau(\eta)$, for arbitrary values of the parameter τ and the argument η. The FD integrals are a class of functions that are used extensively in the modeling of semiconductor devices, e.g., when the charge carriers are in a strongly quantum, degenerate regime, such as in heavily doped semiconductors. The determination of FD integrals has a long history. Our approach to evaluating these functions is two-fold. First, we develop exact power series expansions of the integral. These series, however, converge too slowly to be a practical means of evaluating the integral. The second aspect of our approach is to apply numerical series acceleration methods to improve the rate of convergence of these power series expansions. Indeed, it would not be feasible to use the series expansions without implementing an acceleration method. The result is a computer program that provides efficient, accurate values of the FD integral.

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I. INTRODUCTION

In modeling semiconductor devices, the number of free electrons per unit volume, n, in the conduction band depends on the density of states D(E) available for occupation, and on the Fermi Dirac distribution function $f_{FD}(E)$, which yields the probability that a state of energy E is occupied [Ref. 1: pg. 90]

$$n = \int_{E_c}^{E_t} dED(E) f_{FD}(E) \ . \tag{1}$$

Here, E_c is the conduction band energy lower level, and E_t is the top of the conduction band. The three dimensional form of the density of states, D(E) is [Ref. 1: pg. 91]

$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}\ , \tag{2}$$

where m* is the effective mass of the charge carrier. The Fermi Dirac distribution function is

$$f_{FD}(E) = \frac{1}{1+\exp(\beta(E-\mu))}\ , \tag{3}$$

where β is equal to $(\kappa T)^{-1}$, and μ is the Fermi energy. When E is equal to μ, $f_{FD}(E)$ is equal to 1/2. Combining Eqs. (1-3) n becomes

$$n = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^{E_t - E_c} \frac{dy\sqrt{y}}{1+\exp(\beta(y + E_c - \mu))}\ , \tag{4}$$

where y is equal to $E-E_c$.

Since the upper limit of the energy integral will represent few electrons, setting

(E_t-E_C) equal to infinity, ∞, will introduce an exponentially small error into the value of the integral. This approximation is allowed because $f(E)$ vanishes quickly for energy $E >> \mu$. The equation for the number of carriers per unit volume is then

$$n = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{dy\sqrt{y}}{1+\exp(\beta(y+E_c-\mu))}. \tag{5}$$

We then have

$$n = \frac{1}{2\pi^2}\left(\frac{2m^*}{\beta\hbar^2}\right)^{3/2} F_{1/2}\left(\beta\left(\mu - E_c\right)\right), \tag{6}$$

where $F_{½}$ denotes the following integral

$$F_{1/2}(z) = \int_0^\infty \frac{x^{1/2}}{1+\exp(x-z)}dx. \tag{7}$$

This integral is but one example of an entire family of integrals labeled by the parameter τ in the following manner

$$F_\tau(z) = \int_0^\infty \frac{x^\tau}{1+\exp(x-z)}dx. \tag{8}$$

These integrals are known as Fermi-Dirac integrals. The purpose of this thesis is to examine methods of computing Fermi-Dirac integrals. In the following sections we will use the conventional notation and take the definition of the F-D integral to be the following [Ref. 3: pg. 1067]

$$f_\tau(\eta) = \frac{1}{\Gamma(\tau+1)}F_\tau(\eta) = \frac{1}{\Gamma(\tau+1)}\int_0^\infty \frac{x^\tau}{1+\exp(x-\eta)}dx, \tag{9}$$

where Γ is the standard gamma function [Ref. 2 : Ch. 6]. Returning to the case of the three dimensional electron gas, setting $\tau = 1/2$; and using the fact $\Gamma(3/2)$ becomes $(\pi/2)^{1/2}$, we have

$$n = \frac{1}{\sqrt{2}}\left[\frac{m^* kT}{\pi\hbar^2}\right]^{3/2} f_{1/2}\left(\beta\left(E_c - \mu\right)\right). \tag{10}$$

The equation for n becomes a constant times $f_{1/2}(\beta(E_c-\mu))$, as long as the temperature is invariant.

Thus we see that the carrier density in a semiconductor is generally related to the FD integral function. Except in special cases, the FD integral cannot be evaluated analytically in closed form. In many treatments of the carrier density, the following approximation is adopted. When $\beta(\mu-E_c) << -1$, i.e. when the Fermi level lies at least several multiples of κT below the conduction band, we can approximate $f_{1/2}(y) \sim e^y$ for $y << 0$. We will term this the Boltzmann limit, since in this case the Fermi Dirac distribution goes over to the Boltzmann distribution function. We then recover the often used approximation $n = N_c e^{-\beta(E_c-\mu)}$, where N_c is equal to $\frac{1}{\sqrt{2}}\left(\frac{m^* kT}{\pi\hbar^2}\right)^{3/2}$. However, for accurate modeling of the carrier density in semiconductor, or when the Fermi level lies close to the conduction band edge, we can no longer invoke this approximation. Instead we must evaluate the Fermi-Dirac integral.

When the Fermi level, μ, is close to the conduction band, E_c, the electron gas is considered degenerate. If x, which corresponds to $\beta\mu$, is much greater than one, then the evaluation of the Fermi-Dirac integral must be evaluated in the extreme quantum or strong degeneracy regime. Accurate evaluations for the FD integral in the extreme quantum

region can be done with well known techniques, such as the *Ehrenburg, Joyce-Dixon, Chang-Izabelle*, or the *Nilsson* approximations [Ref. 1: pp. 111-114]. However, in the intermediate semi-classical regime, neither the Boltzmann or the strong degenerate approximations are applicable.

The semi-classical regime is of particular importance to the field of semiconductor physics, where the controlled doping of the intrinsic material can range from the classic to the strong degenerate regime. Attempts to evaluate the FD in the past have included tables of values by McDougall and Stoner (1938) [Ref. 7] for the range $-4 \leq x \leq 20$, in increments of $\Delta x = 0.1$. Entries were accurate to seven digits for τ equal to 1/2 and 3/2, and five digit accuracy for $\tau = -1/2$. Rhodes (1950) [Ref. 8] provided formulas and tables of $F_\tau(x)$, for $\tau = 1, 2, 3$, and 4 in the interval $|x| \leq 4.0$. A parallel effort has been made to develop approximants which can replicate the values of the Fermi-Dirac integrals, $f_\tau(x)$ to exemplary accuracy for different ranges of x. Whereas tabular data is used in conjunction with interpolation methods; by incorporating an approximate formula within an algorithm, the values of F_τ can be calculated directly by the user.

In terms of the analytical treatment of $F_\tau(x)$ the code developed by Dingle (1957) [Ref. 9] is quite valuable. His work has provided the portion of an FD integral that was discarded in Sommerfield's (1928) [Ref. 10] treatment of the extreme quantum regime. Especially effective approximants were given by Code and Thatcher (1967) [Ref. 11] for $\tau = -1/2, 1/2, 3/2$, and by Van Halen and Pulfrey (1985) [Ref. 12] for $\tau = -1/2, 1/2, 312, 5/2, 3$, and 7/2. [Ref. 3: pg. 1071]. Blakemore has provided reference and tabulated material; [Ref. 4: Appendix B] and summarized much of the data on Fermi Dirac integrals through 1981 [Ref. 3]

In view of the continuing need to generate accurate values for Fermi Dirac integrals for arbitrary values of x, we were motivated to reexamine this subject and to develop an efficient algorithm that delivers precise values. Our program can be employed to generate directly the values of desired FD integrals, or to generate tables of highly accurate values which can then be used in conjunction with standard interpolation methods.

Our approach, rather than following the route of numerical integration adopted by McDougall and Stoner, consists of utilizing exact series expansions of $f_\tau(x)$ .The apparent difficulty that a given expansion converges very slowly is overcome by the powerful series acceleration method of Levin [Ref. 5] , that will be covered in Chapter III. To obtain very high accuracy in the value of a slowly converging series, it turns out to be sufficient to input into the Levin method only the first fifteen terms of a given series expansion.

In Chapter II we summarize several known formulas for FD integrals which apply for the integer values of τ. This is followed by the derivation of exact series expansion of an FD integral, which can be used in conjunction with the Levin series acceleration method for general values of τ, as discussed in Chapter III. Without the aid of a series acceleration method, the various formulas we give would, from an practical view, be ineffective throughout the interval $-1 \leq x \leq 10$. This underscores the great usefulness of the Levin method for the evaluation of the general Fermi Dirac integral. Finally, Chapter IV summarizes our results. In the appendices we present our algorithm, Blakemore's tabulated data for the half integer values of τ, and a comparison of our values to Blakemore's in the region of $-4 \leq x \leq 4$, for different values of half integer τ.

The necessity to understand the importance of Fermi-Dirac integrals is imperative in the modeling of semiconductor devices. For example in the determination of n, the number of charge carriers, $\tau = 1/2$ is used to model a three dimensional semiconductor. In the case of a two dimensional electron gas, found, for example, in the channel of a MOSFET device, the effective density of states must be changed to $Nc = m^*/(\pi \hbar^2 \beta)$ and τ will be equal to 0. For a one dimensional electron gas, found in modern "quantum wire" devices, N_c is equal to $[m^*/(\pi \hbar^2 \beta)]^{-1/2}$ and τ is equal to - 1/2 [Ref. 1: Ch. 3]. We note that these values of τ for a D-dimensional electron gas, $\tau = (D-2)/2$, arise from the assumption of a parabolic band structure function $E(k) = \hbar^2 k^2/2m^*$, appropriate to free particles. When one includes a more realistic, nonparabolic band structure, such as is required for PbTe, PbSe, and PbS; then n turns out to be given by a linear combination of $f_{3/2}(\eta)$ and $f_{5/2}(\eta)$ [Ref. 6: pg. 47]. In this thesis we include the values of $f_\tau(x)$ for $\tau = 7/2$, in order to have full comparison with Blakemore's tabulated data. In this age of miniaturization of semiconductor devices the applicability of the Boltzmann approximation will soon be exhausted. The ability to accurately model the number of free electrons will require the utilization of numerical algorithms. Also, in the future, if the need arises to find the Fermi-Dirac integrals of an arbitrary value of τ, the program we present will be capable.

II. ANALYTICAL METHODS

In the first part of this chapter we list several known, convenient formulas, for $f_\tau(x)$ which apply for integer values of τ. This is followed by exact series expansions for FD integrals for general τ in the separate regime of positive and negative values of x. The expansion we give for $x > 0$ is new. When used with the Levin method, these expansions can provide values which are correct to not less than six significant figures for any value of the argument. Throughout this thesis we restrict our attention to real values of x.

For $\tau = 0$ one can evaluate the FD integral in closed form, $f_0(x) = \ln(1+e^x)$. Starting with this result and repeatedly invoking the relationship $\partial f_\tau / \partial x = f_{\tau-1}$, one can derive explicit formulas for $f_\tau(x)$ for τ equal to any negative integer. Formulas for τ equal to a positive integer can be obtain from f_0 by repeated integrations, but the evaluation of these integrals in closed form can not be achieved.

For negative values of x, for arbitrary τ, there exists the convergent expansion

$$f_\tau(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^{\tau+1}} e^{nx} \quad , (x<0). \tag{11}$$

This result is arrived at by simply substituting the geometric series expansion into Eq. (9):

$$\frac{e^{x-s}}{1+e^{x-s}} = \sum_{n=1}^{\infty} (-1)^{n+1} e^{n(x-s)} \quad , \tag{12}$$

which converges for all $s \geq 0$ as long as $x \leq 0$, and integrating term by term. For the special case $x = 0$ we have

$$f_\tau(0) = \eta(\tau+1), \tag{13}$$

where $\eta(s)$ is defined for any positive integer s by [Ref. 2: Ch. 23]

$$\eta(s) = \sum_{m1}^{\infty} (-1)^{m+1} / m^s \quad . \tag{14}$$

Because of the frequent occurrence of the quantity η(s) in the treatment of the general FD integral, we summarize its major properties. It is closely related to the Rieman zeta function, ζ(s) defined by

$$\zeta(s) = \sum_{m=1}^{\infty} 1/m^s \quad . \tag{15}$$

Specifically one has [Ref. 2: Ch. 23]

$$\eta(s) = \left(1 - \frac{1}{2^s - 1}\right)\zeta(s) \, . \tag{16}$$

Highly accurate values for the η(s) are given in Table 23.3 of reference 2 and can easily be reproduced by using the Levin method. The latter route was used within the ANSI C code used in our algorithm.

It should be noted that the series on the right hand side of Eq. (14) converges only if the Re s > 0, as should be expected since the expansion given by Eq. (11) for $f_\tau(x)$ is similarly restricted. Even though the expansion in Eq. (11) converges for $x \leq 0$, for numerical purposes it is nominally useful only if $x \leq -1$, because the rate of convergence of the series decreases sharply as x approaches 0 from below. In practice this equation is useful within the interval $-1 \leq x \leq 0$ only if the method of Levin is used .

For $x > 0$ it is useful to rewrite f as the sum of two integrals, the first extending from 0 to x and the second extending from x to ∞. In the first of these intervals we change of variable $s = x(1-y)$ and use the identity $1/(e^{-xy}+1) = 1-1/(e^{xy}+1)$. In the second integral we change variable, $s = x(1+y)$ This gives

$$f_\tau(x) = \frac{x^{\tau+1}}{\Gamma(\tau+2)}\left\{1+(\tau+1)\left[A_\tau(x)-B_\tau(x)\right]\right\}, \tag{17}$$

where the functions $A_\tau(X)$ and $B_\tau(x)$ are defined by the relations

$$A_\tau(x) = \int_0^\infty dy \frac{(1+y)^\tau}{e^{xy}+1}, \tag{18}$$

$$B_\tau(x) = \int_0^1 dy \frac{(1-y)^\tau}{e^{xy}+1}. \tag{19}$$

Note that the integral in Eq. (18) converges as long as $x > 0$, whereas the integral in equation (19) converges for positive and negative values of x.

Before presenting our method for evaluating these functions we summarize their analytical properties and derive several useful expansion formulas. If τ is a positive integer or zero, the function $A_\tau(x)$ has an isolated pole at $x = 0$ of degree $\tau+1$. This can be seen directly by making the change of variable $u = xy$. For all other non-integer values of τ, $A_\tau(x)$ has an isolated branch point at $x = 0$. The leading behavior for small positive x is obtained by noting that in this regime the convergence of the integral is achieved by the growth of the exponential term for values of y satisfying the inequality $y >> 1/x$, for which the numerator in equation (18) can be approximated by y^τ. Thus, for very small positive values of x we have the result $A_\tau(x) \sim Cx^{-(\tau+1)}$, where $C = \Gamma(\tau + 1)\eta(\tau + 1)$. The full expansion for small x is fairly involved and we shall not give it here.

A far more useful expansion is provided by the following. We expand $e^{-xy}/(1 + e^{-xy})$ as a geometric series in powers of e^{-xy}, which converges for all positive values of x, utilize Eq (13.2.5) of reference 2,

$$\int_0^\infty dy(1+y)^\tau e^{-xy} = \mathrm{U}(1,\ 2+\tau,\ \mathrm{x}), \tag{20}$$

where U denotes the standard irregular solution of the confluent hypergeometric equation. The major properties of this function are listed in Chapter 13 of reference 2. The final result is

$$A_\tau(x) = \sum_{k=1}^{\infty} (-1)^k \mathrm{U}(1,\ 2\ +\ \tau,\ \mathrm{x})\ . \tag{21}$$

We have found that the simplest way to evaluate the U functions appearing in this equation accurately is to use the continued fraction representation

$$\mathrm{U}(1,\ 2\ +\ \tau,\ z) = \frac{1|}{|z} + \frac{(-\tau)|}{|1} + \frac{1|}{|z} + \frac{1-\tau|}{|1} + \frac{2|}{|z} + \frac{2-\tau|}{|1} + \frac{3|}{|z} + \ldots. \tag{22}$$

This representation converges for all z. In fact, the rate of convergence is greater the larger the value of |z| If expanded in powers of 1/z, the result is the standard asymptotic expansion, i.e. Eq. (13 .5 .2) of reference 2

$$\mathrm{U}(1,\ 2+\tau,\ z) \sim \sum_{n=0}^{\infty} (-\tau)_n (-z)^{-(n+1)}\ . \tag{23}$$

Here $(z)_n$ is the Pochammer symbol defined by $z_0 = 1$, $z_n = (z + 1)...(z\ + n - 1)$ for n = 1, 2, ... Note that, whereas the asymptotic expansion diverges for all z, the continued fraction expansion, equation (22), converges for all z.

Returning to the series in equation (21), for large values of the argument kx, the function U(1, 2 + τ, kx) decreases to zero as 1/(kx). As such, the series in question is only conditionally convergent. The direct method of summing the series as it stands is impractical, because if one were to sum the first N terms the resulting error in the estimate of the infinite series would only be of order of the last term retained, i.e. *O(1/N).* However, although this expansion is slowly convergent, it can be evaluated to very high

accuracy using the Levin method, and then it is necessary to evaluate only the fifteen or so terms of the series in equation (21).

We now discuss some of the properties of the function $B_\tau(x)$. As remarked earlier, the integral in Eq. (19) converges for both positive and negative real values of x. In fact, with the aid of the identity $1/(e^{-xy} + 1) = 1 - 1/(e^{xy} + 1)$ one finds that

$$B_\tau(x) + B_\tau(-x) = 1/(\tau + 1) . \tag{24}$$

The singularities of $B_\tau(x)$ closest to the origin in the complex x plane are the pair of branch points at $\pm i\pi$, as can be seen from the fact that for these choices of x the integrand in Eq. (19) has simple poles for y = 1. Hence $B_\tau(x)$ admits a convergent Maclaurin expansion within the circle of radius π centered about the origin. The form of the Maclaurin expansion is readily established. We substitute into Eq. (19) the expansion

$$\frac{1}{e^{xy}+1} = \frac{1}{2} - \sum_{n=1}^{\infty} \frac{(2^{2n}-1)B_{2n}x^{2n-1}}{n\Gamma(\tau+1+2n)} , \tag{25}$$

which converges for real values of y in the interval [0, 1] as long as $|x| < \pi$. The quantities B_{2n} are the Bernoulli numbers, referred to above. One thus arrives at the Maclaurin expansion

$$B_\tau(x) = \frac{1}{2(\tau+1)} - \frac{\Gamma(\tau+1)}{2} \sum_{n=1}^{\infty} \frac{\left(2^{2n}-1\right)B_{2n}x^{2n-1}}{n\Gamma\left(\tau+1+2n\right)} . \tag{26}$$

Although one can utilize this expansion along with the Levin method to obtain accurate values for values of x somewhat beyond $x = \pi$, a different type of expansion is necessary for larger x. In the following we provide a far more effective expansion. The derivation starts from the definition, Eq. (19), and we utilize Eq. (13.2.1) of reference 2,

$$\int_0^1 dy(1-y)^{\tau} e^{-xy} = \left[1/(\tau+1) \right] M(1,\ 2+\tau,-x)\ , \tag{27}$$

where M denotes the usual confluent hypergeometric function,

$$M(a,c,z)\ = \sum_{k=0}^{\infty} \frac{(a)_k}{k!(c)_k} z^k\ . \tag{28}$$

In this way we arrive at

$$B_{\tau}(x) = [1/(\tau+1)] \sum_{k=1}^{\infty} (-1)^{k+1} M(1,2+\tau,-kx). \tag{29}$$

Upon utilizing the asymptotic property [Ref. 2: Eq. (13.1.5)]

$$M(a,\ c,\ z) = [\Gamma(c)/\Gamma(c\text{-}a)](-z)^{-a}[1+O(1/z)]\ \ (\mathrm{Re}\ z < 0), \tag{30}$$

one notes that the typical term of the series, including the factor $(-1)^{k+1}$, decreases to zero for large values of k proportional to $(-1)^{k+1}/k$. It thus follows that the series in Eq.(29) is conditionally convergent for all positive values of x. As in the case of the series, Eq.(21), for $A_{\tau}(x)$, the Levin method can be used with great effectiveness for this conditionally convergent series.

To evaluate the confluent hypergeometric functions $M(1,\ 2+\tau,\ -kx)$ appearing in Eq.(26) accurately, two routes are open. One method consists of exploiting the Kummer identity [Ref. 2: Eq. (13.1.27)],

$$M(a,\ c,\ z) = e^{z} M(c\text{-}a,\ c,\ -z), \tag{31}$$

so that evaluation of $B_{\tau}(x)$ would proceed by invoking the Levin method on the series

$$B_{\tau}(x) = [\ 1/(\tau+1\ )] \sum_{k=1}^{\infty} (-1)^{k+1} e^{-kx} M(1+\tau,2+\tau,kx)\ , \tag{32}$$

A second, more effective, method for evaluating M is to use the continued fraction representation

$$M(1, c, z) = \frac{1|}{|1} - \frac{z|}{|c} + \frac{z|}{|c+1} - \frac{cz|}{|c+2} + \frac{2z|}{|c+3} - \frac{(c+1)z|}{|c+4} + \ldots \quad (33)$$

which converges for all finite z. Once accurate values of the first fifteen terms of the series in Eq. (32) are computed, the application of the Levin method to these terms of the series provides estimates of $B_\tau(x)$ of very high accuracy.

In the following chapter we digress to provide a brief description of the Levin method and the conditions to be met in order for the method to be effective. We will show that these conditions are met for all of the expansions encountered in this work. In Chapter IV we display some numerical results obtained using the present method and discuss the accuracy that can be achieved.

III. SERIES ACCELERATION METHOD

In this chapter we shall present a brief description of the Levin series acceleration method, the key formulas, as well as a list of conditions to be met for the method to be effective Although, the method first appeared in print over two decades ago, it is still virtually unknown in the physics community. This method is for many classes of problems perhaps the most effective technique currently available to accelerate the convergence of a series. For further details on the general method the reader can consult Levin's original paper [Ref. 5].

The central goal is, given a quantity T represented by an infinite series, to obtain highly accurate estimates of the value of that quantity utilizing only the first few terms of the series. To fix the notation, let the individual terms of the infinite series be denoted by t_n so that

$$T = \sum_{n=1}^{\infty} t_n \quad . \tag{34}$$

We will require values of the partial sums, T_n (n = 1,2,3,...), of the infinite series, which are defined by

$$T_n = \sum_{k=1}^{n} t_k \quad . \tag{35}$$

In the following, we explicitly consider the vast class of infinite series with the property that the error in approximating T by the value of the partial sum T_n , is of order the last individual term retained, t_n. As discussed below, this class includes convergent as well as divergent series. A quantitative statement of this property is provided by the relation

$$T_n = T + t_n g_n, \tag{36}$$

for all positive integers n, where g_n possesses a unique, finite limit for $n\to\infty$. Now the sequence $\{g_n\}$ will possess this property as long as the ratios of successive terms of the given series, namely t_n/t_{n+1} , approach a unique finite limit, differing from unity, for $n\to\infty$. To prove this, note that from Eq. (36) we have

$$g_{n+1} = 1 + g_n\left[\frac{t_n}{t_{n+1}}\right]. \tag{37}$$

We now suppose that the ratio in parenthesis in Eq (37) has a unique limit, ξ, such that

$$\xi = \lim_{n\to\infty}(t_n / t_{n+1}) \tag{38}$$

exists. It thus follows from Eq. (37) and (38) that

$$g_\infty = \lim_{n\to\infty} g_n = \frac{1}{1-\xi} \tag{39}$$

We therefore arrive at the claimed result that, if ξ exists and is unique and is unequal to unity, the sequence $\{g_n\}$ possesses a unique limit for $n \to \infty$, given by Eq. (39).

It is important to note that Eqs. (37) and (38) can apply even if the infinite series representation of T diverges. For example, for the terms of the infinite series in Eq (11), which converge only if $x < 0$ one has $\xi = -e^{-x}$ so that $g_\infty = 1/(1+e^{-x})$. In particular, the quantity g_∞ exists and is finite for both positive and negative values of x. Similarly, the infinite series representation of T can be a divergent asymptotic series, arrived at, for example, by formal expansion of a portion of the integrand of a bona fide integral representation of T.

Now, the Levin method consists of adopting the assumption that g_n is well approximated by a polynomial in 1/n. We define a series of approximations $g_n[N]$ to the true g_n defined in Eq. (36), by the following,

$$g_n[N] = \sum_{k=0}^{N-2} c_k (1/n)^k \,, \tag{40}$$

where N denotes the Nth Levin approximant. Inspecting Eq. (40) one can anticipate that this basic assumption of the Levin method will be appropriate if t_n/t_{n+1} is a slowly varying function of 1/n. Adopting Eq. (36) we proceed to require that for a fixed value of N, T_n = T[N] + g_n[N] for n = 1, 2, ...,N. Here T[N] denotes the Levin estimates of T as obtained by employing Eq. (36) and the first N terms of the series of Eq. (34) . We now have N equations which determine the N unknown quantities T[N], $\{c_k\}$, (k = 0, 1, 2, .., N-2). It turns out that T[N] is given by

$$T[N] = P[N]/Q[N] \tag{41}$$

Where

$$P[N] = \sum_{k=1}^{N} (-1)^k k^{N-1} (T_k / t_k) N!/[k!(N-k)!] \tag{42}$$

and

$$Q[N] = \sum_{k=1}^{N} (-1)^k k^{N-1} (1/t_k) N!/[k!(N-k)!] \tag{43}$$

We reiterate, the Levin estimates for the value of the infinite series T, which utilize the first N terms of the series, is given by equations (41-43). This estimate can be expected to serve as a good approximation for T in those cases where the ratios of successful terms, t_n/t_{n+1}, is a slowly varying function of 1/n. In this regard for the series expansions of an FD integral which have appeared in Chapter II, (Eqs. 11, 21, 26, 29, and 32) the ratios of successive terms are in fact slowly varying in 1/n.

In practice where deployment of the method is justified, the estimates T[N] for N equal to 13, 14, or 15 typically are very nearly equal, and the first set of common digits

can be taken as providing a reliable estimate of the value of the infinite series T. It is frequently impractical to consider larger values of N because the individual terms of the series in Eqs. (42) and (43) become so large the severe round off problems arise in the course of summing the series.

For example, the value $\eta(1)$ is ln(2) or 0.693147805599453 [Ref. 2]. By using Eq. (14) and summing the first 15 terms the value of $\eta(1)$ is quickly resolved. As can be seen

i	T[i]	t[i]	P[i]/Q[i]
1	1.000000	1.000000	1.0000000000000000
2	0.500000	-0.500000	0.6666666666666666
3	0.833333	0.333333	0.6944444444444444
4	0.583333	-0.250000	0.6931372549019607
5	0.783333	0.200000	0.6931439393939393
6	0.616667	-0.166667	0.6931474019283138
7	0.759524	0.142857	0.6931471777900349
8	0.634524	-0.125000	0.6931471800150043
9	0.745635	0.111111	0.6931471806012292
10	0.645635	-0.100000	0.6931471805592412
11	0.736544	0.090909	0.6931471805598541
12	0.653211	-0.083333	0.6931471805599531
13	0.730134	0.076923	0.6931471805599453
14	0.658705	-0.071429	0.6931471805599453
15	0.725372	0.066667	0.6931471805599454

Table 1

in the table 1 by the fifteenth term in the series there is agreement with the accepted value of ln(2) out to the 16th decimal place. If one one directly summed the series representation of $\eta()$, Eq. (14), it would take significantly more than fifteen terms to reach this level of accord. In fact we used the first billion terms in Eq. (14) and reached agreement only to the fourth decimal place. The exercise required two hours of CPU time on a SPARC 10 Sun workstation. Clearly using the series acceleration method of Levin is the proper course of action when summing these types of series.

IV. RESULTS

The algorithm was built as a set of subroutines to be called by the parent equation. For example Eq. (17) requires a gamma function. In turn the Eqs. (18) and (19) that are called by Eq. (17) require hypergeometric and confluent hypergeometric functions. These subroutine were tested against known values in reference 2. Once the gamma, hypergeometric, confluent hypergeometric and eta functions were working perfectly they were combined to get the desired Eqs. (17), (18) and (19).

Next we ran the algorithm from the interval $-4 \leq x \leq 4$ to replicate the tabulated data in Blakemore. The values of τ that were of interest were the half integer values -1/2, 1/2, 3/2, 5/2, and 7/2. In Figures 1- 5 we show the error of our code as compared to Blakemore's data. The error was calculated by the formula [(B-L)/B]*100 to get a percentage, where B is Blakemore's value and L is the output of our algorithm. It is obvious from inspection of the figures that the accord with Blakemore's data is to the last digit. We, of course, claim that our results are more accurate than published results of Blakemore; because of suspected round off error in his results. The flow of data, as a function of x, is shown in Figure 6, where the Blakemore values are plotted as straight lines and F(x), the output of our program is superimposed with circles. In order to fully represent the values of our data tabulated comparison to Blakemore's values are collected in Appendix C. It is quite clear that we had agreement with Blakemore to the last digit for $f_\tau(x)$ for all the values of x . The strength of this program is the speed of the Levin method. In the fraction of a minute all the values of $f_\tau(x)$ were generated between $-4 \leq x \leq 4$.

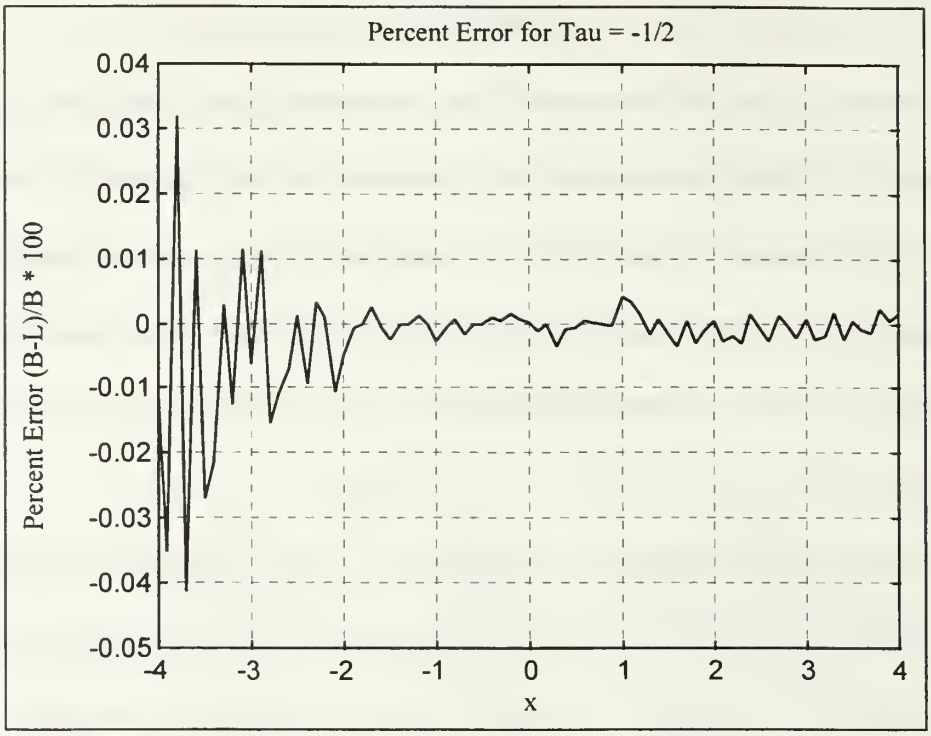

Figure 1: Percent Error for $\tau = -1/2$

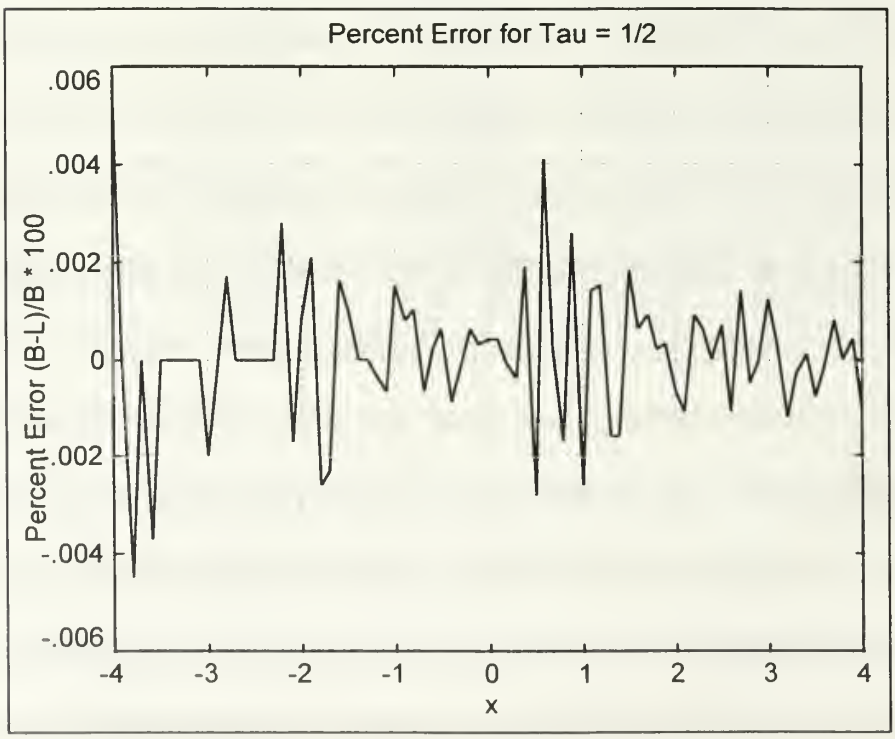

Figure 2: Percent Error for $\tau = 1/2$

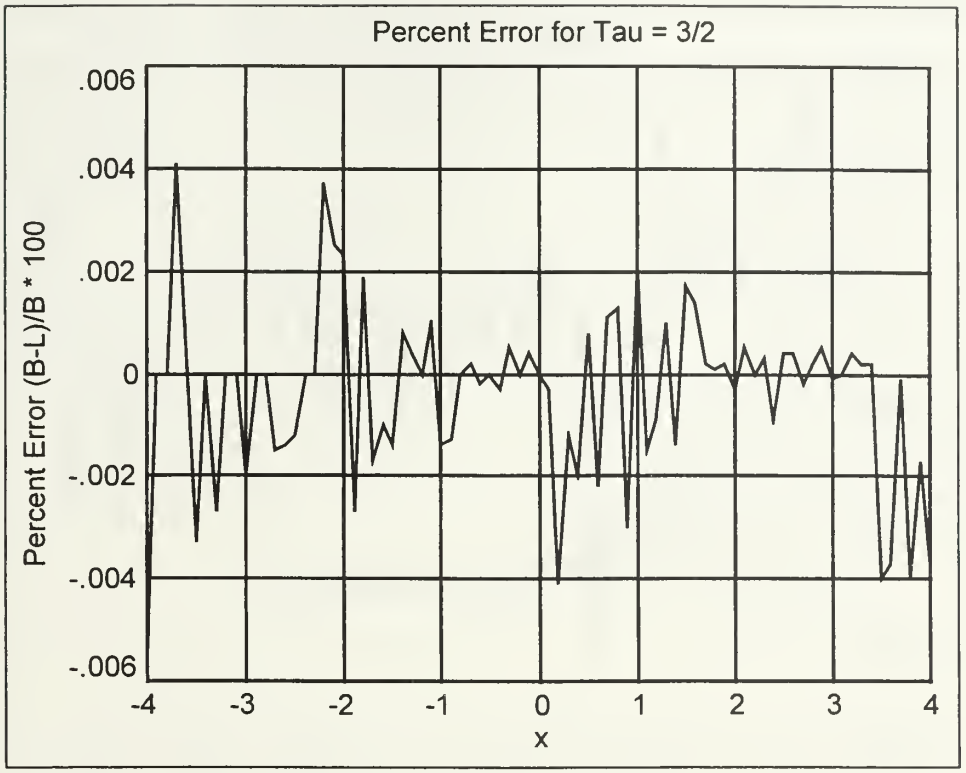

Figure 3: Percent Error for $\tau = 3/2$

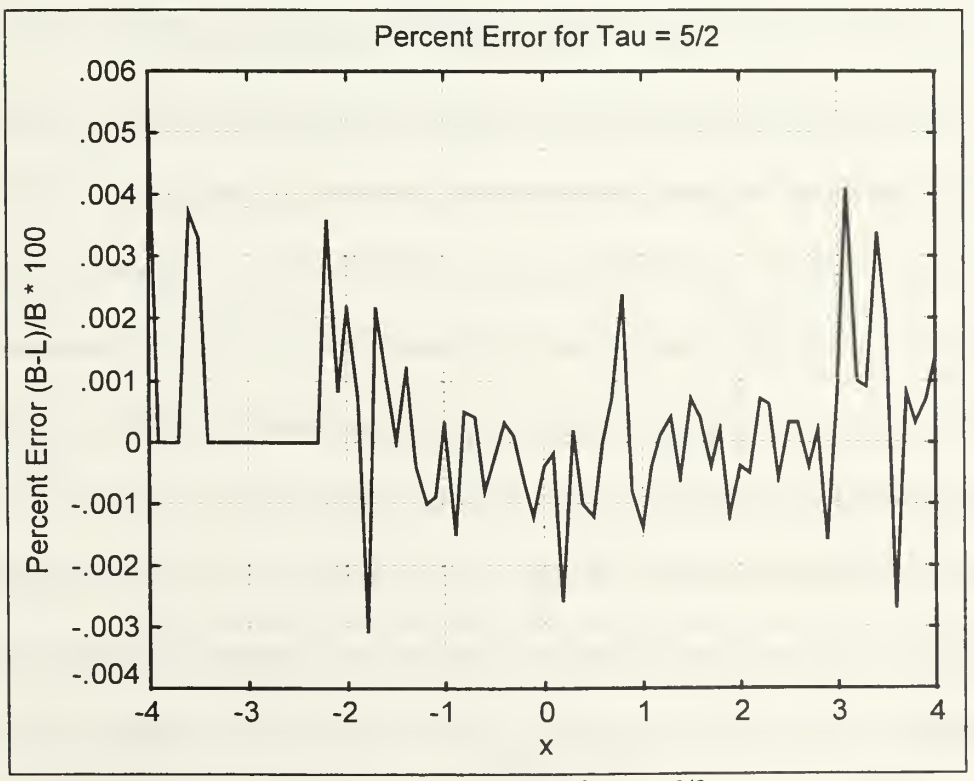

Figure 4: Percent Error for $\tau = 5/2$

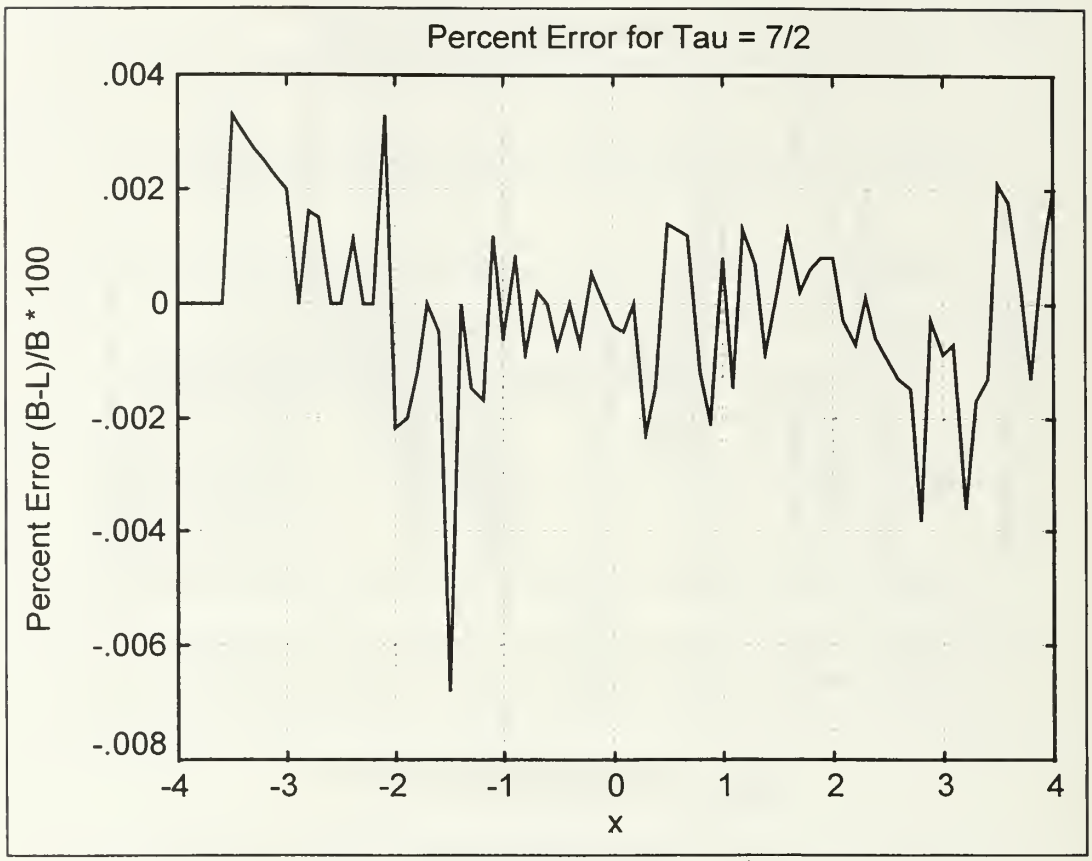

Figure 5: Percent Error for $\tau = 7/2$

Prior to using the method of Levin we tried to duplicate the results by letting the infinite series run until they were in agreement in the sixteen decimal place. This proved to be taxing on both machine and programmer. Once the jobs were completed there was poor agreement with accept value as shown in Figure 7 for $\tau = 1/2$. This fluctuation about the accepted value of $f_\tau(x)$ is due to round off error in summing the infinite series. Since the algorithm ran for days there was plenty of time and opportunity for errors to build up and truncate through the iteration. For other values of τ the disparity between accepted and calculated values were just as poor for values of $x > 0$. Therefore in order for series approximations to be useful in the modeling of FD integral, the use of series accelerations methods such as Levin is paramount.

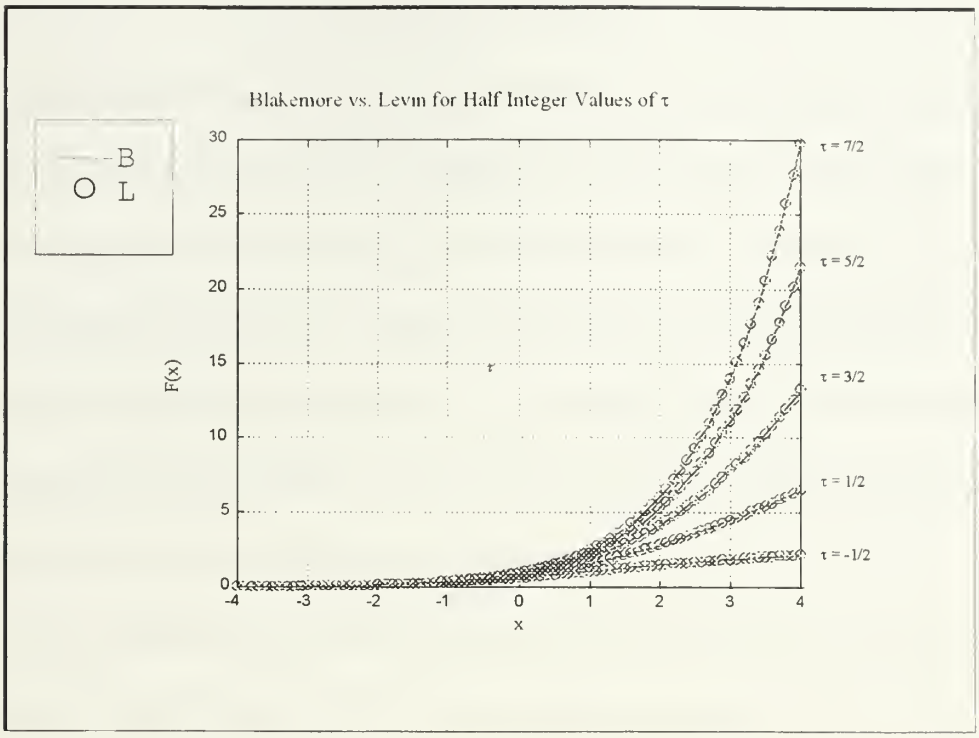

Figure 6: Comparison of Levin to Blakemore for half integer values of τ

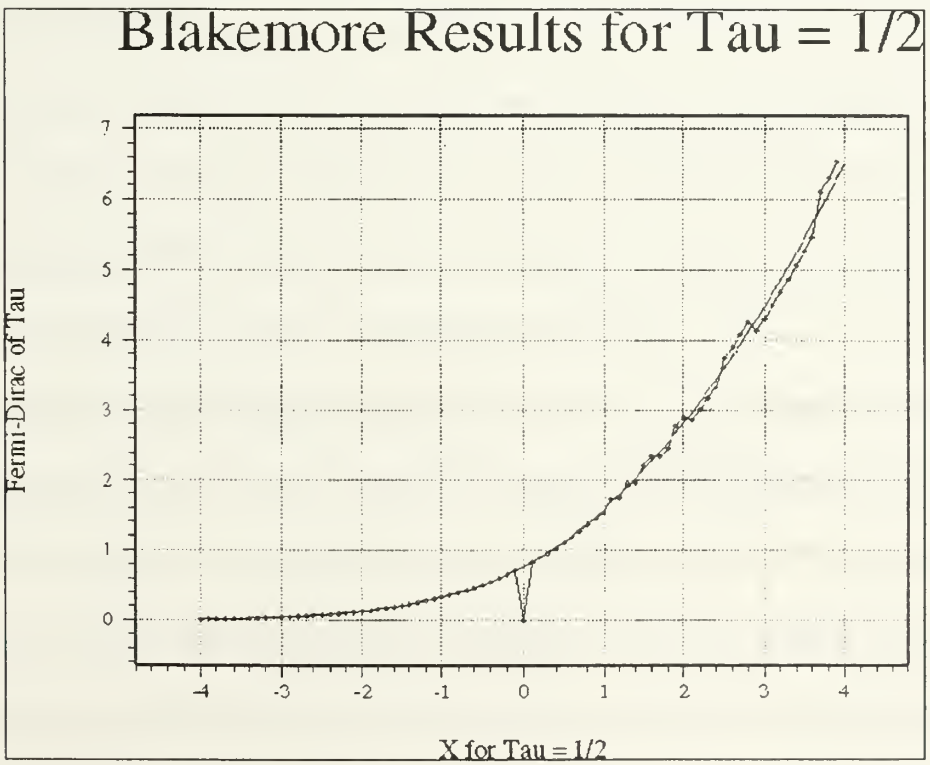

Figure 7: Illustration of the error generated when the Levin Method is not used

V. CONCLUSIONS

In this thesis we have developed a new, highly efficient algorithm for evaluating Fermi-Dirac (FD) integrals, $f_\tau(x)$, the definition of which is given in equation (9). Fermi-Dirac integrals are widely used in numerous aspects of semiconductor modeling, as we have discussed in Chapter I. Except in special cases, FD integrals cannot be given in closed form using elementary functions. There has been a long history of attempts to provide methods for approximately evaluating these integrals. The algorithm developed in this thesis is based on the following two-fold approach.

First, we employ various series expansions, derived in Chapter II starting from the definition of the FD integral. For $x < 0$, for example, we employ the expansion given by equation (11). For $x > 0$, however, we utilize equation (17), which in turn is evaluated using the series expansions given by equations (21) and (29). These expansions provide an alternate, exact representation of the Fermi-Dirac integral, each applicable in its respective domain of validity. While these expansions are mathematically exact, their utility is seemingly limited since their rate of convergence is typically so slow as to render them impractical as a means of evaluating FD integrals.

The second part of our approach, therefore, is to use a novel series acceleration method as applied to the expansions derived in Chapter II. The general aspects of this method, due originally to Levin, Ref. [5], are discussed in Chapter III. An illustration of the power of the Levin method was given in Chapter III. There, we applied the series acceleration method to the evaluation of the eta function, defined by the power series given in equation (14). This expansion converges too slowly, to the point where

straightforward summation of (14) is futile, since, as the series is an alternating series, round-off errors ultimately limit computational accuracy. Summation of a billion terms in Eq. (14) produced only 4 digits of accuracy. Application of the Levin technique, however, readily produced 16 digit accuracy in only 16 iterations of the method.

The results we obtain by applying the Levin method to the exact series expansions of the FD integrals are discussed in Chapter IV. We have compared our calculated results with those tabulated in the book by Blakemore, Ref. [4], which is a standard in the literature of semiconductor modeling. In Figure 6 we show Blakemore's results in the solid curves; are our results indicated with circles. On the scale of Figure 6 it would appear there is perfect agreement. Blakemore, however, only cites values of FD integrals to four significant digits. In Figures 1-5, we illustrate percentage error of our results as compared with those of Blakemore. In all cases our results agree with those of Blakemore to the number of digits that Blakemore lists.

We believe our work sets a new benchmark for the computation of FD integrals. We note that while the most useful FD integrals are those with the parameter τ restricted to half-integer values (i.e., τ = -1/2, 1/2, 3/2, etc.), our algorithm can evaluate FD integrals with arbitrary values of τ, a feature not previously available to the best of our knowledge. From a practical point of view, one could envision two uses of the algorithm developed here. First, the algorithm could be developed as a sub-routine to be embedded in a larger device simulation code. In the accurate modeling of PN junctions, for example, especially those utilizing heavily doped semiconductor regions (as in Esaki diodes), one needs to make repeated calls to a general function that evaluates the FD

integrals. If such function calls become too numerous, however, one might envision the use of our algorithm as follows. One would use the sub-routine to first evaluate the FD integral over a range of values. These values would then be stored as a look-up table, to which standard numerical interpolation methods would then be applied.

```
/*Thesis Program to solve Fermi-Dirac Intergrals with the method of Levine*/
/*Lt. Jeremy Thompson*/
/*Compiler: Boreland Turbo C++*/
/*File Name: fd.c*/
#include<stdio.h>
#include<math.h>
#include<stdlib.h>
#define MAX 15
double inpvar(double);
void print_results(double, double);
double eta(double);                    /* In accordance with (IAW) Eq. 16*/
double eq11(double, double);
double hypo(double,double,double);     /* IAW Eq. 22*/
double gamma(double);
double eq18(double,double);
void fermdir(double);
double contfrac(double,double);        /*Eq. 33*/
double eq32(double,double);
double fact(double);
double levin();
double bico(int,int);                  /* Ref. 13*/
double factln(int n);
double gammln(float xx);

double T[MAX+1],t[MAX+1];

void main()
        {double tau;
        tau=inpvar(tau);
        fermdir(tau);
        return;}

double inpvar(double tau)
        {printf("\n What is the value of tau ?\n");
        scanf("%lf",&tau);
        return tau;}

void print_results(double x, double fx)
        {printf("%lf \t%34.32lf \n",x,fx);
        return;}

void fermdir(double tau)
        {double x,fx,a,b;
        x=-4.0;
        while(x<4.1)
                {if(x<0.0)
                        {fx=eq11(x,tau);}
                if(fabs(x)<.01)
                        {fx=eta(tau+1.0);}
                if(x>=.1)
                        {a=fx=eq18(tau,x);
                        b=eq32(tau,x);
                        fx=fx-b;
                        fx=1+(tau+1)*fx;
```

```
                    fx=fx*pow(x,tau+1);
                    fx=fx/gamma(tau+2);}
        print_results(x,fx);
        x=x+0.1;}
        return;}

double eq11(double x, double tau)
        {double y;
        int n,k;
        T[0]=t[0]=0.0;
        n=k=1;
        y=pow(-1,n+1)*exp(n*x)/(pow(n,tau+1));
        while(k<=MAX)
                {t[k]=pow(-1,n+1)*exp(n*x)/(pow(n,tau+1));
                T[k]=T[k-1]+t[k];
                n=n+1;
                k=k+1;}
                y=levin();
        return y;}

double hypo(double a,double c,double z)
        {long double a1,c1,z1,temp,kfact;
        double m;
        int k;
        k=0;a1=a;c1=c;kfact=1;temp=0;
        m=1;z1=z;
        while(fabs(m-temp)>1e-14)
                {k=k+1;
                kfact=kfact*k;
                temp=m;
                        if(k<=1)
                        {m=m+(a/c*z1/kfact);}
                        else
                        {a=a*(a1+k-1);
                        c=c*(c1+k-1);
                        m=m+(a/c*z1/kfact);
                }
                z1=z1*z;}
        return m;}

double gamma (double tau)
        {double y,temptau,gammatau,temp;
         y=tau;
         temptau=1.0000;
                while(tau>2)
                {tau=tau-1;
                temptau=temptau*tau;
                }
                while(tau<-2)
                {tau=tau+1;
                temptau=temptau/(tau-1);
                }
        gammatau=1.0000000*pow(tau,1);                          /* Ref. 2*/
        gammatau = gammatau + (0.5772156649015329*pow(tau,2));
```

```
        gammatau = gammatau + (-.6558780715202538*pow(tau,3));
        gammatau = gammatau + (-.4200260350340952*pow(tau,4));
        gammatau = gammatau + (0.1665386113822915*pow(tau,5));
        gammatau = gammatau + (-.4219777345555443*pow(tau,6));
        gammatau = gammatau + (-.0096219715278770*pow(tau,7));
        gammatau = gammatau + (0.0072189432466630*pow(tau,8));
        gammatau = gammatau + (-.0011651675918591*pow(tau,9));
        gammatau = gammatau + (-.0002152416741149*pow(tau,10));
        gammatau = gammatau + (0.0001280502823882*pow(tau,11));
        gammatau = gammatau + (-.0000201348547807*pow(tau,12));
        gammatau = gammatau + (-.0000012504934821*pow(tau,13));
        gammatau = gammatau + (0.0000011330272320*pow(tau,14));
        gammatau = gammatau + (-.0000002056338417*pow(tau,15));
        gammatau = gammatau + (0.0000000061160950*pow(tau,16));
        gammatau = gammatau + (0.0000000050020075*pow(tau,17));
        gammatau = gammatau + (-.0000000011812746*pow(tau,18));
        gammatau = gammatau + (0.0000000001043427*pow(tau,19));
        gammatau = gammatau + (0.0000000000077823*pow(tau,20));
        gammatau = gammatau + (-.0000000000036968*pow(tau,21));
        gammatau = gammatau + (0.0000000000005100*pow(tau,22));
        gammatau = gammatau + (-.0000000000000206*pow(tau,23));
        gammatau = gammatau + (-.0000000000000054*pow(tau,24));
        gammatau = gammatau + (0.0000000000000014*pow(tau,25));
        gammatau = gammatau + (0.0000000000000001*pow(tau,26));
        tau=y;
        y=(1/gammatau)*temptau;
        return y;}

double eq18 (double tau, double x)
        {double a;
        int k;T[0]=t[0]=0.0;
        k=1;
        while(k<=MAX)
        {t[k]=pow(-1,k)*contfrac(2+tau,k*x);
    T[k]=T[k-1]+t[k];k=k+1;}
        a=levin();
        return fabs(a);}

double contfrac(double tau, double z)
        {double a[1000],b[1000],value,old;
        int i,k,index;
        index=0;
    tau=tau-2;
        k=0;
        while(k<1000)
                {a[k]=b[k]=0;k++;}
    k=0;
        a[1]=1;b[1]=z;
        for(i=2;i<=999;++i)
                {if(k<1)
                        {a[i]=index-tau;
                        b[i]=1;
                        index=index+1;
                        k=2;}
```

```
                else
                        {a[i]=index;
                        b[i]=z;
                        k=0;}
                }
        i=1;old=a[i]/b[i];
        i=2;value=a[i]/b[i];
        i=i-1;value=a[i]/(b[i]+value);
        i=2;
        while(fabs(value-old)>1e-16)
                {old=value;
                i=i+1;
                index=i;
                value=a[i]/b[i];
                while(index>1)
                        {index=index-1;
                        value=a[index]/(b[index]+value);}
                }
        return value;}

double eq32(double tau,double x)
        {double value;
        int k; k=1; T[0]=t[0]=0.0;
        while(k<=MAX)
    {t[k]=pow(-1,k+1)*exp(-k*x)*hypo(1+tau,2+tau,k*x);
         T[k]=T[k-1]+t[k];k=k+1;}
        value=levin();
        value=value/(tau+1);
    return value;}

double levin()
        {double P[MAX+1],Q[MAX+1];
        int l;l=1;
        while(l<=MAX)
        {P[l]=P[l-1]+pow(-1,l)*pow(l,MAX-1)*T[l]/t[l]*bico(MAX,l);
         Q[l]=Q[l-1]+pow(-1,l)*pow(l,MAX-1)/t[l]*bico(MAX,l);
        l=l+1;}
        return (P[MAX]/Q[MAX]);}

double fact(double k)
        {double kfact;
        kfact=1;
        while(k>1)
        {kfact=kfact*k;k--;}
    return kfact;}

double eta(double s)
        {double temp;
        int m;m=1;
        while(m<=MAX)
        {T[m]=T[m-1]+pow(-1,m+1)/pow(m,s);
        t[m]=pow(-1,m+1)/pow(m,s);
        m=m+1;}
        temp=levin();
```

```
        return temp;}

double bico(int n, int k)                                   /* Ref. 13*/
        {double factln(int n);
        return floor(0.5+exp(factln(n)-factln(k)-factln(n-k)));
        }

double factln(int n)                                        /* Ref. 13*/
        {double gammln(float xx);
        static float a[101];
        if (n <= 1) return 0.0;
        if (n <= 100) return a[n] ? a[n] : (a[n]=gammln(n+1.0));
        else return gammln(n+1.0);
        }

double gammln(float xx)                                     /* Ref. 13*/
        {double x,y,tmp,ser;
        static double cof[6]={76.18009172947146,-86.50532032941677,
                24.01409824083091,-1.231739572450155,
                0.1208650973866179e-2,-0.5395239384953e-5};
        int j;
        y=x=xx;
        tmp=x+5.5;
        tmp -= (x+0.5)*log(tmp);
        ser=1.000000000190015;
        for (j=0;j<=5;j++) ser += cof[j]/++y;
        return -tmp+log(2.5066282746310005*ser/x);}
```

APPENDIX B. BLAKEMORE'S TABULATED VALUES FOR HALF INTEGER VALUES OF $f_\tau(x)$

x	-0.5	0.5	1.5	2.5	3.5
-4.0	0.01808	0.018199	0.018256	0.018287	0.018301
-3.9	0.01995	0.020099	0.02017	0.020206	0.020224
-3.8	0.02203	0.022195	0.022283	0.022327	0.022349
-3.7	0.02429	0.02451	0.024617	0.02467	0.024697
-3.6	0.02681	0.027063	0.027193	0.027259	0.027291
-3.5	0.02956	0.02988	0.030037	0.030118	0.030158
-3.4	0.0326	0.032986	0.033179	0.033276	0.033325
-3.3	0.03595	0.036412	0.036645	0.036764	0.036824
-3.2	0.03962	0.040187	0.040473	0.040617	0.040690
-3.1	0.04367	0.044349	0.044696	0.044872	0.044961
-3.0	0.0481	0.048933	0.049356	0.049571	0.049679
-2.9	0.05298	0.053984	0.054498	0.054759	0.054891
-2.8	0.05831	0.059545	0.06017	0.060488	0.060649
-2.7	0.06417	0.065665	0.066425	0.066813	0.067009
-2.6	0.07059	0.072398	0.073323	0.073795	0.074033
-2.5	0.07762	0.079804	0.080927	0.081501	0.081791
-2.4	0.08529	0.087944	0.089309	0.090006	0.090360
-2.3	0.09369	0.096887	0.098544	0.099391	0.099822
-2.2	0.10284	0.10671	0.10872	0.10975	0.11027
-2.1	0.1128	0.11748	0.11992	0.12117	0.12181
-2.0	0.12366	0.1293	0.13225	0.13377	0.13454
-1.9	0.13546	0.14225	0.14581	0.14766	0.14860
-1.8	0.14829	0.15642	0.16074	0.16297	0.16412
-1.7	0.162	0.17193	0.17714	0.17986	0.18125
-1.6	0.177	0.18889	0.19517	0.19846	0.20015
-1.5	0.1933	0.2074	0.21497	0.21895	0.22099
-1.4	0.21074	0.22759	0.23671	0.24152	0.24401
-1.3	0.229	0.24959	0.26055	0.26636	0.26938
-1.2	0.24958	0.27353	0.28669	0.2937	0.29736
-1.1	0.27108	0.29955	0.31533	0.32378	0.32822
-1.0	0.29402	0.3278	0.34667	0.35686	0.36222
-0.9	0.318	0.35841	0.38096	0.39321	0.39970
-0.8	0.34438	0.39154	0.41844	0.43316	0.44098
-0.7	0.37181	0.42733	0.45936	0.47702	0.48646
-0.6	0.40077	0.46595	0.504	0.52515	0.53653
-0.5	0.43123	0.50754	0.55265	0.57795	0.59164
-0.4	0.46318	0.55224	0.60561	0.63583	0.65229
-0.3	0.49657	0.60022	0.66321	0.69923	0.71899
-0.2	0.53137	0.65161	0.72577	0.76863	0.79234
-0.1	0.5675	0.70654	0.79365	0.84455	0.87294
0.0	0.6049	0.76515	0.8672	0.92755	0.96148

x	-0.5	0.5	1.5	2.5	3.5
0.0	0.6049	0.76515	0.8672	0.92755	0.96148
0.1	0.64348	0.82756	0.9468	1.0182	1.05870
0.2	0.68317	0.89388	1.0328	1.1171	1.16540
0.3	0.72382	0.96422	1.1257	1.225	1.28240
0.4	0.7654	1.0387	1.2258	1.3425	1.41070
0.5	0.80774	1.1173	1.3336	1.4704	1.55130
0.6	0.85074	1.2003	1.4494	1.6095	1.70520
0.7	0.89429	1.2875	1.5738	1.7606	1.8736
0.8	0.93826	1.3791	1.7071	1.9246	2.0577
0.9	0.98255	1.4752	1.8497	2.1023	2.2589
1.0	1.0271	1.5756	2.0023	2.2948	2.4787
1.1	1.0717	1.6806	2.165	2.5031	2.7184
1.2	1.1163	1.79	2.3385	2.7282	2.9799
1.3	1.1608	1.9038	2.5232	2.9712	3.2647
1.4	1.2052	2.0221	2.7194	3.2332	3.5747
1.5	1.2493	2.1449	2.9278	3.5155	3.9120
1.6	1.2931	2.272	3.1486	3.8192	4.2786
1.7	1.3366	2.4035	3.3823	4.1456	4.6766
1.8	1.3796	2.5393	3.6294	4.4961	5.1085
1.9	1.4222	2.6794	3.8903	4.8719	5.5767
2.0	1.4643	2.8237	4.1654	5.2746	6.0838
2.1	1.5058	2.9722	4.4552	5.7055	6.6325
2.2	1.5468	3.1249	4.76	6.1662	7.2258
2.3	1.5872	3.2816	5.0803	6.658	7.8668
2.4	1.6271	3.4423	5.4164	7.1827	8.5585
2.5	1.6663	3.607	5.7689	7.7419	9.3044
2.6	1.7049	3.7755	6.138	8.3371	10.108
2.7	1.743	3.948	6.5241	8.97	10.973
2.8	1.7804	4.1241	6.9277	9.6425	11.903
2.9	1.8172	4.304	7.3491	10.356	12.903
3.0	1.8535	4.4876	7.7886	11.113	13.976
3.1	1.8891	4.6747	8.2467	11.915	15.127
3.2	1.9242	4.8653	8.7237	12.763	16.360
3.3	1.9588	5.0595	9.2199	13.66	17.681
3.4	1.9927	5.2571	9.7357	14.608	19.094
3.5	2.0262	5.458	10.271	15.608	20.605
3.6	2.0591	5.6623	10.827	16.662	22.218
3.7	2.0915	5.8699	11.404	17.774	23.939
3.8	2.1235	6.0806	12.001	18.944	25.774
3.9	2.1549	6.2945	12.62	20.175	27.730
4.0	2.1859	6.5115	13.26	21.469	29.812

APPENDIX C. TABULATED COMPARISON TO BLAKEMORE'S DATA FOR HALF INTEGER VALUES OF τ

Tau = -0.5

x	Blakemore	Levine	Per Cent Error	x	Blakemore	Levine	Per Cent Error
-4.0	0.01808	0.018082	-0.0111%	0.1	0.64348	0.643488	-0.0012%
-3.9	0.01995	0.019957	-0.0351%	0.2	0.68317	0.68317	0.0000%
-3.8	0.02203	0.022023	0.0318%	0.3	0.72382	0.723846	-0.0036%
-3.7	0.02429	0.0243	-0.0412%	0.4	0.7654	0.765408	-0.0010%
-3.6	0.02681	0.026807	0.0112%	0.5	0.80774	0.807746	-0.0007%
-3.5	0.02956	0.029568	-0.0271%	0.6	0.85074	0.850744	-0.0005%
-3.4	0.0326	0.032607	-0.0215%	0.7	0.89429	0.894288	0.0002%
-3.3	0.03595	0.035949	0.0028%	0.8	0.93826	0.938262	-0.0002%
-3.2	0.03962	0.039625	-0.0126%	0.9	0.98255	0.982555	-0.0005%
-3.1	0.04367	0.043665	0.0114%	1.0	1.0271	1.027057	0.0042%
-3.0	0.0481	0.048103	-0.0062%	1.1	1.0717	1.071666	0.0032%
-2.9	0.05298	0.052974	0.0113%	1.2	1.1163	1.116284	0.0014%
-2.8	0.05831	0.058319	-0.0154%	1.3	1.1608	1.16082	-0.0017%
-2.7	0.06417	0.064177	-0.0109%	1.4	1.2052	1.205192	0.0007%
-2.6	0.07059	0.070595	-0.0071%	1.5	1.2493	1.249323	-0.0018%
-2.5	0.07762	0.077619	0.0013%	1.6	1.2931	1.293147	-0.0036%
-2.4	0.08529	0.085298	-0.0094%	1.7	1.3366	1.336605	-0.0004%
-2.3	0.09369	0.093687	0.0032%	1.8	1.3796	1.379643	-0.0031%
-2.2	0.10284	0.102839	0.0010%	1.9	1.4222	1.422219	-0.0013%
-2.1	0.1128	0.112812	-0.0106%	2.0	1.4643	1.464295	0.0003%
-2.0	0.12366	0.123666	-0.0049%	2.1	1.5058	1.50584	-0.0027%
-1.9	0.13546	0.135461	-0.0007%	2.2	1.5468	1.546831	-0.0020%
-1.8	0.14826	0.14826	0.0000%	2.3	1.5872	1.587248	-0.0030%
-1.7	0.16213	0.162126	0.0025%	2.4	1.6271	1.627078	0.0014%
-1.6	0.17712	0.177121	-0.0006%	2.5	1.6663	1.666313	-0.0008%
-1.5	0.1933	0.193305	-0.0026%	2.6	1.7049	1.704946	-0.0027%
-1.4	0.21074	0.21074	0.0000%	2.7	1.743	1.742977	0.0013%
-1.3	0.22948	0.22948	0.0000%	2.8	1.7804	1.780408	-0.0004%
-1.2	0.24958	0.249577	0.0012%	2.9	1.8172	1.817241	-0.0023%
-1.1	0.27108	0.27108	0.0000%	3.0	1.8535	1.853485	0.0008%
-1.0	0.29402	0.294028	-0.0027%	3.1	1.8891	1.889147	-0.0025%
-0.9	0.31845	0.318452	-0.0006%	3.2	1.9242	1.924237	-0.0019%
-0.8	0.34438	0.344378	0.0006%	3.3	1.9588	1.958767	0.0017%
-0.7	0.37181	0.371816	-0.0016%	3.4	1.9927	1.992748	-0.0024%
-0.6	0.40077	0.400771	-0.0002%	3.5	2.0262	2.026194	0.0003%
-0.5	0.43123	0.431231	-0.0002%	3.6	2.0591	2.059117	-0.0008%
-0.4	0.46318	0.463176	0.0009%	3.7	2.0915	2.091532	-0.0015%
-0.3	0.49657	0.496568	0.0004%	3.8	2.1235	2.123453	0.0022%
-0.2	0.53137	0.531362	0.0015%	3.9	2.1549	2.154894	0.0003%
-0.1	0.5675	0.567496	0.0007%	4.0	2.1859	2.18587	0.0014%
0.0	0.6049	0.604899	0.0002%				

Table C1: Comparison to Blakemore's data to the Levinized values in the interval $-4 \leq x \leq 4$ for $\tau = -1/2$.

Tau = 0.5

x	Blakemore	Levine	Per Cent Error	x	Blakemore	Levine	Per Cent Error
-4.0	0.018199	0.018198	0.0055%	0.1	0.82756	0.827557	0.0004%
-3.9	0.020099	0.020099	0.0000%	0.2	0.89388	0.893881	-0.0001%
-3.8	0.022195	0.022196	-0.0045%	0.3	0.96422	0.964224	-0.0004%
-3.7	0.02451	0.02451	0.0000%	0.4	1.0387	1.03868	0.0019%
-3.6	0.027063	0.027064	-0.0037%	0.5	1.1173	1.117331	-0.0028%
-3.5	0.02988	0.02988	0.0000%	0.6	1.2003	1.200251	0.0041%
-3.4	0.032986	0.032986	0.0000%	0.7	1.2875	1.287498	0.0002%
-3.3	0.036412	0.036412	0.0000%	0.8	1.3791	1.379123	-0.0017%
-3.2	0.040187	0.040187	0.0000%	0.9	1.4752	1.475161	0.0026%
-3.1	0.044349	0.044349	0.0000%	1.0	1.5756	1.575641	-0.0026%
-3.0	0.048933	0.048934	-0.0020%	1.1	1.6806	1.680576	0.0014%
-2.9	0.053984	0.053984	0.0000%	1.2	1.79	1.789974	0.0015%
-2.8	0.059545	0.059544	0.0017%	1.3	1.9038	1.903831	-0.0016%
-2.7	0.065665	0.065665	0.0000%	1.4	2.0221	2.022133	-0.0016%
-2.6	0.072398	0.072398	0.0000%	1.5	2.1449	2.144861	0.0018%
-2.5	0.079804	0.079804	0.0000%	1.6	2.272	2.271987	0.0006%
-2.4	0.087944	0.087944	0.0000%	1.7	2.4035	2.403478	0.0009%
-2.3	0.096887	0.096887	0.0000%	1.8	2.5393	2.539294	0.0002%
-2.2	0.10671	0.106707	0.0028%	1.9	2.6794	2.679391	0.0003%
-2.1	0.11748	0.117482	-0.0017%	2.0	2.8237	2.823721	-0.0007%
-2.0	0.1293	0.129299	0.0008%	2.1	2.9722	2.972233	-0.0011%
-1.9	0.14225	0.142247	0.0021%	2.2	3.1249	3.124871	0.0009%
-1.8	0.15642	0.156424	-0.0026%	2.3	3.2816	3.28158	0.0006%
-1.7	0.17193	0.171934	-0.0023%	2.4	3.4423	3.442301	-0.0000%
-1.6	0.18889	0.188887	0.0016%	2.5	3.607	3.606975	0.0007%
-1.5	0.2074	0.207398	0.0010%	2.6	3.7755	3.775543	-0.0011%
-1.4	0.22759	0.22759	0.0000%	2.7	3.948	3.947945	0.0014%
-1.3	0.24959	0.24959	0.0000%	2.8	4.1241	4.124119	-0.0005%
-1.2	0.27353	0.273531	-0.0004%	2.9	4.304	4.304006	-0.0001%
-1.1	0.29955	0.299552	-0.0007%	3.0	4.4876	4.487547	0.0012%
-1.0	0.3278	0.327795	0.0015%	3.1	4.6747	4.674684	0.0003%
-0.9	0.35841	0.358407	0.0008%	3.2	4.8653	4.865358	-0.0012%
-0.8	0.39154	0.391536	0.0010%	3.3	5.0595	5.059513	-0.0003%
-0.7	0.42733	0.427333	-0.0007%	3.4	5.2571	5.257093	0.0001%
-0.6	0.46595	0.465949	0.0002%	3.5	5.458	5.458044	-0.0008%
-0.5	0.50754	0.507537	0.0006%	3.6	5.6623	5.662314	-0.0002%
-0.4	0.55224	0.552245	-0.0009%	3.7	5.8699	5.869851	0.0008%
-0.3	0.60022	0.600221	-0.0002%	3.8	6.0806	6.080604	-0.0000%
-0.2	0.65161	0.651606	0.0006%	3.9	6.2945	6.294526	-0.0004%
-0.1	0.70654	0.706538	0.0003%	4.0	6.5115	6.511568	-0.0010%
0.0	0.76515	0.765147	0.0004%				

Table C2: Comparison to Blakemore's data to the Levinized values in the interval $-4 \leq x \leq 4$ for $\tau = 1/2$.

Tau = 3/2

x	Blakemore	Levine	Per Cent Error	x	Blakemore	Levine	Per Cent Error
-4.0	0.018256	0.018257	-0.0055%	0.1	0.9468	0.946803	-0.0003%
-3.9	0.02017	0.02017	0.0000%	0.2	1.0328	1.032842	-0.0041%
-3.8	0.022283	0.022283	0.0000%	0.3	1.1257	1.125713	-0.0012%
-3.7	0.024617	0.024616	0.0041%	0.4	1.2258	1.225824	-0.0020%
-3.6	0.027193	0.027193	0.0000%	0.5	1.3336	1.333589	0.0008%
-3.5	0.030037	0.030038	-0.0033%	0.6	1.4494	1.449432	-0.0022%
-3.4	0.033179	0.033179	0.0000%	0.7	1.5738	1.573783	0.0011%
-3.3	0.036645	0.036646	-0.0027%	0.8	1.7071	1.707078	0.0013%
-3.2	0.040473	0.040473	0.0000%	0.9	1.8497	1.849755	-0.0030%
-3.1	0.044696	0.044696	0.0000%	1.0	2.0023	2.002258	0.0021%
-3.0	0.049356	0.049357	-0.0020%	1.1	2.165	2.165032	-0.0015%
-2.9	0.054498	0.054498	0.0000%	1.2	2.3385	2.338522	-0.0009%
-2.8	0.06017	0.06017	0.0000%	1.3	2.5232	2.523175	0.0010%
-2.7	0.066425	0.066426	-0.0015%	1.4	2.7194	2.719437	-0.0014%
-2.6	0.073323	0.073324	-0.0014%	1.5	2.9278	2.927749	0.0017%
-2.5	0.080927	0.080928	-0.0012%	1.6	3.1486	3.148555	0.0014%
-2.4	0.089309	0.089309	0.0000%	1.7	3.3823	3.382292	0.0002%
-2.3	0.098544	0.098544	0.0000%	1.8	3.6294	3.629395	0.0001%
-2.2	0.10872	0.108716	0.0037%	1.9	3.8903	3.890294	0.0002%
-2.1	0.11992	0.119917	0.0025%	2.0	4.1654	4.165414	-0.0003%
-2.0	0.13225	0.132247	0.0023%	2.1	4.4552	4.455178	0.0005%
-1.9	0.14581	0.145814	-0.0027%	2.2	4.76	4.759999	0.0000%
-1.8	0.16074	0.160737	0.0019%	2.3	5.0803	5.080287	0.0003%
-1.7	0.17714	0.177143	-0.0017%	2.4	5.4164	5.416448	-0.0009%
-1.6	0.19517	0.195172	-0.0010%	2.5	5.7689	5.768879	0.0004%
-1.5	0.21497	0.214973	-0.0014%	2.6	6.138	6.137973	0.0004%
-1.4	0.23671	0.236708	0.0008%	2.7	6.5241	6.524116	-0.0002%
-1.3	0.26055	0.260551	-0.0004%	2.8	6.9277	6.927688	0.0002%
-1.2	0.28669	0.28669	0.0000%	2.9	7.3491	7.349063	0.0005%
-1.1	0.31533	0.315327	0.0010%	3.0	7.7886	7.788611	-0.0001%
-1.0	0.34667	0.346675	-0.0014%	3.1	8.2467	8.246693	0.0000%
-0.9	0.38096	0.380965	-0.0013%	3.2	8.7237	8.723665	0.0004%
-0.8	0.41844	0.41844	0.0000%	3.3	9.2199	9.21988	0.0002%
-0.7	0.45936	0.459361	-0.0002%	3.4	9.7357	9.735682	0.0002%
-0.6	0.504	0.504001	-0.0002%	3.5	10.271	10.271411	-0.0040%
-0.5	0.55265	0.55265	0.0000%	3.6	10.827	10.827402	-0.0037%
-0.4	0.60561	0.605612	-0.0003%	3.7	11.404	11.403983	0.0001%
-0.3	0.66321	0.663207	0.0005%	3.8	12.001	12.001479	-0.0040%
-0.2	0.72577	0.72577	0.0000%	3.9	12.62	12.620209	-0.0017%
-0.1	0.79365	0.793647	0.0004%	4.0	13.26	13.260488	-0.0037%
0.0	0.8672	0.8672	0.0000%				

Table C3: Comparison to Blakemore's data to the Levinized values in the interval $-4 \leq x \leq 4$ for $\tau = 3/2$.

Tau = 5/2

x	Blakemore	Levine	Per Cent Error	x	Blakemore	Levine	Per Cent Error
-4.0	0.018287	0.018286	0.0055%	0.1	1.0182	1.018202	-0.0002%
-3.9	0.020206	0.020206	0.0000%	0.2	1.1171	1.117129	-0.0026%
-3.8	0.022327	0.022327	0.0000%	0.3	1.225	1.224998	0.0002%
-3.7	0.02467	0.02467	0.0000%	0.4	1.3425	1.342513	-0.0010%
-3.6	0.027259	0.027258	0.0037%	0.5	1.4704	1.470418	-0.0012%
-3.5	0.030118	0.030117	0.0033%	0.6	1.6095	1.6095	0.0000%
-3.4	0.033276	0.033276	0.0000%	0.7	1.7606	1.760588	0.0007%
-3.3	0.036764	0.036764	0.0000%	0.8	1.9246	1.924554	0.0024%
-3.2	0.040617	0.040617	0.0000%	0.9	2.1023	2.102316	-0.0008%
-3.1	0.044872	0.044872	0.0000%	1.0	2.2948	2.294833	-0.0014%
-3.0	0.049571	0.049571	0.0000%	1.1	2.5031	2.50311	-0.0004%
-2.9	0.054759	0.054759	0.0000%	1.2	2.7282	2.728197	0.0001%
-2.8	0.060488	0.060488	0.0000%	1.3	2.9712	2.971187	0.0004%
-2.7	0.066813	0.066813	0.0000%	1.4	3.2332	3.233219	-0.0006%
-2.6	0.073795	0.073795	0.0000%	1.5	3.5155	3.515476	0.0007%
-2.5	0.081501	0.081501	0.0000%	1.6	3.8192	3.819185	0.0004%
-2.4	0.090006	0.090006	0.0000%	1.7	4.1456	4.145618	-0.0004%
-2.3	0.099391	0.099391	0.0000%	1.8	4.4961	4.496089	0.0002%
-2.2	0.10975	0.109746	0.0036%	1.9	4.8719	4.871957	-0.0012%
-2.1	0.12117	0.121169	0.0008%	2.0	5.2746	5.274622	-0.0004%
-2.0	0.13377	0.133767	0.0022%	2.1	5.7055	5.705528	-0.0005%
-1.9	0.14766	0.147659	0.0007%	2.2	6.1662	6.166159	0.0007%
-1.8	0.16297	0.162975	-0.0031%	2.3	6.658	6.658043	-0.0006%
-1.7	0.17986	0.179856	0.0022%	2.4	7.1827	7.182746	-0.0006%
-1.6	0.19846	0.198458	0.0010%	2.5	7.7419	7.741875	0.0003%
-1.5	0.21895	0.21895	0.0000%	2.6	8.3371	8.337077	0.0003%
-1.4	0.24152	0.241517	0.0012%	2.7	8.97	8.970038	-0.0004%
-1.3	0.26636	0.266361	-0.0004%	2.8	9.6425	9.642481	0.0002%
-1.2	0.2937	0.293703	-0.0010%	2.9	10.356	10.356169	-0.0016%
-1.1	0.32378	0.323783	-0.0009%	3.0	11.113	11.1129	0.0009%
-1.0	0.35686	0.356859	0.0003%	3.1	11.915	11.914509	0.0041%
-0.9	0.39321	0.393216	-0.0015%	3.2	12.763	12.762868	0.0010%
-0.8	0.43316	0.433158	0.0005%	3.3	13.66	13.659883	0.0009%
-0.7	0.47702	0.477018	0.0004%	3.4	14.608	14.607497	0.0034%
-0.6	0.52515	0.525154	-0.0008%	3.5	15.608	15.607684	0.0020%
-0.5	0.57795	0.577952	-0.0003%	3.6	16.662	16.662454	-0.0027%
-0.4	0.63583	0.635828	0.0003%	3.7	17.774	17.773851	0.0008%
-0.3	0.69923	0.699229	0.0001%	3.8	18.944	18.943948	0.0003%
-0.2	0.76863	0.768635	-0.0007%	3.9	20.175	20.174854	0.0007%
-0.1	0.84455	0.84456	-0.0012%	4.0	21.469	21.468708	0.0014%
0.0	0.92755	0.927554	-0.0004%				

Table C4: Comparison to Blakemore's data to the Levinized values in the interval $-4 \leq x \leq 4$ for $\tau = 5/2$.

Tau = 7/2

x	Blakemore	Levine	Per Cent Error	x	Blakemore	Levine	Per Cent Error
-4.0	0.018301	0.018301	0.0000%	0.1	1.0587	1.058705	-0.0005%
-3.9	0.020224	0.020224	0.0000%	0.2	1.1654	1.1654	0.0000%
-3.8	0.022349	0.022349	0.0000%	0.3	1.2824	1.282429	-0.0023%
-3.7	0.024697	0.024697	0.0000%	0.4	1.4107	1.410721	-0.0015%
-3.6	0.027291	0.027291	0.0000%	0.5	1.5513	1.551278	0.0014%
-3.5	0.030158	0.030157	0.0033%	0.6	1.7052	1.705177	0.0013%
-3.4	0.033325	0.033324	0.0030%	0.7	1.8736	1.873578	0.0012%
-3.3	0.036824	0.036823	0.0027%	0.8	2.0577	2.057724	-0.0012%
-3.2	0.04069	0.040689	0.0025%	0.9	2.2589	2.258948	-0.0021%
-3.1	0.044961	0.04496	0.0022%	1.0	2.4787	2.478679	0.0008%
-3.0	0.049679	0.049678	0.0020%	1.1	2.7184	2.71844	-0.0015%
-2.9	0.054891	0.054891	0.0000%	1.2	2.9799	2.979861	0.0013%
-2.8	0.060649	0.060648	0.0016%	1.3	3.2647	3.264676	0.0007%
-2.7	0.067009	0.067008	0.0015%	1.4	3.5747	3.574733	-0.0009%
-2.6	0.074033	0.074033	0.0000%	1.5	3.912	3.911994	0.0002%
-2.5	0.081791	0.081791	0.0000%	1.6	4.2786	4.278543	0.0013%
-2.4	0.09036	0.090359	0.0011%	1.7	4.6766	4.676589	0.0002%
-2.3	0.099822	0.099822	0.0000%	1.8	5.1085	5.108468	0.0006%
-2.2	0.11027	0.11027	0.0000%	1.9	5.5767	5.576653	0.0008%
-2.1	0.12181	0.121806	0.0033%	2.0	6.0838	6.083752	0.0008%
-2.0	0.13454	0.134543	-0.0022%	2.1	6.6325	6.632518	-0.0003%
-1.9	0.1486	0.148603	-0.0020%	2.2	7.2258	7.225849	-0.0007%
-1.8	0.16412	0.164122	-0.0012%	2.3	7.8668	7.866792	0.0001%
-1.7	0.18125	0.18125	0.0000%	2.4	8.5585	8.558551	-0.0006%
-1.6	0.20015	0.200151	-0.0005%	2.5	9.3044	9.304489	-0.0010%
-1.5	0.22099	0.221005	-0.0068%	2.6	10.108	10.10812	-0.0013%
-1.4	0.24401	0.24401	0.0000%	2.7	10.973	10.97316	-0.0015%
-1.3	0.26938	0.269384	-0.0015%	2.8	11.903	11.90345	-0.0038%
-1.2	0.29736	0.297365	-0.0017%	2.9	12.903	12.90303	-0.0003%
-1.1	0.32822	0.328216	0.0012%	3.0	13.976	13.97612	-0.0009%
-1.0	0.36222	0.362222	-0.0006%	3.1	15.127	15.12710	-0.0007%
-0.9	0.3997	0.399697	0.0008%	3.2	16.36	16.36058	-0.0036%
-0.8	0.44098	0.440984	-0.0009%	3.3	17.681	17.68130	-0.0017%
-0.7	0.48646	0.486459	0.0002%	3.4	19.094	19.09424	-0.0013%
-0.6	0.53653	0.53653	0.0000%	3.5	20.605	20.60455	0.0021%
-0.5	0.59164	0.591645	-0.0008%	3.6	22.218	22.2176	0.0018%
-0.4	0.65229	0.65229	0.0000%	3.7	23.939	23.93893	0.0003%
-0.3	0.71899	0.718995	-0.0007%	3.8	25.774	25.77432	-0.0013%
-0.2	0.79234	0.792336	0.0005%	3.9	27.73	27.72975	0.0009%
-0.1	0.87294	0.872939	0.0001%	4.0	29.812	29.81139	0.0020%
0.0	0.96148	0.961484	-0.0004%				

Table C5: Comparison to Blakemore's data to the Levinized values in the interval $-4 \leq x \leq 4$ for $\tau = 7/2$.

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